LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100521\
Data File : VU045167.D
Acq On : 06 Oct 2021 00:20
Operator : SY/MD
Sample : M3996-14
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 36 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F4A29

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 0 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Title : VOC Analysis

Signal : TIC: VU045167.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.488	35	46	60	rBV2	70935	206746	15.87%	1.488%
2	1.604	75	82	94	rVB2	187534	215314	16.53%	1.550%
3	1.913	171	178	192	rVB	145244	192436	14.77%	1.385%
4	1.996	195	204	219	rVB	189374	265261	20.36%	1.909%
5	2.205	264	269	286	rVB	20745	30798	2.36%	0.222%
6	2.472	344	352	363	rVB	15792	24621	1.89%	0.177%
7	2.572	370	383	401	rBV	258926	478513	36.74%	3.444%
8	3.048	516	531	537	rBV	60664	124345	9.55%	0.895%
9	3.369	614	631	660	rVB	205105	475683	36.52%	3.424%
10	3.703	723	735	748	rVB5	7094	15944	1.22%	0.115%
11	3.845	769	779	786	rVB4	1075	1738	0.13%	0.013%
12	3.986	808	823	839	rBV4	4277	10529	0.81%	0.076%
13	4.096	844	857	873	rVB5	6435	15756	1.21%	0.113%
14	4.179	873	883	891	rBV3	986	1723	0.13%	0.012%
15	4.301	908	921	923	rBV3	3360	5412	0.42%	0.039%
16	4.443	948	965	978	rBV3	22678	56735	4.36%	0.408%
17	4.536	979	994	1009	rVV2	59848	142457	10.94%	1.025%
18	4.633	1010	1024	1061	rVB	162204	458445	35.20%	3.300%
19	4.990	1123	1135	1144	rBV6	1557	3721	0.29%	0.027%
20	5.070	1144	1160	1175	rBV	229269	498949	38.31%	3.591%
21	5.391	1242	1260	1272	rBV4	68157	171870	13.19%	1.237%
22	5.465	1273	1283	1303	rVB2	83939	192995	14.82%	1.389%
23	5.597	1306	1324	1333	rBV3	24537	55163	4.24%	0.397%
24	5.729	1346	1365	1376	rBV2	478183	1302548	100.00%	9.375%
25	5.854	1393	1404	1410	rBV3	45810	95210	7.31%	0.685%
26	6.134	1480	1491	1506	rVB7	5398	11588	0.89%	0.083%
27	6.253	1511	1528	1565	rBV	379453	756421	58.07%	5.444%
28	6.404	1565	1575	1585	rBV5	4108	7307	0.56%	0.053%
29	6.465	1585	1594	1601	rBV5	3381	5262	0.40%	0.038%
30	6.697	1651	1666	1677	rBV	303071	605279	46.47%	4.356%
31	6.871	1711	1720	1729	rVV3	11439	20718	1.59%	0.149%
32	6.928	1730	1738	1747	rVV2	5962	9841	0.76%	0.071%
33	6.986	1747	1756	1769	rVB7	7768	15688	1.20%	0.113%
34	7.182	1800	1817	1827	rBV9	8809	23072	1.77%	0.166%
35	7.260	1827	1841	1857	rVB	70937	142761	10.96%	1.027%
36	7.334	1857	1864	1865	rBV3	1722	1500	0.12%	0.011%

LSC Area Percent Report

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Operator : SY/MD
Sample : M3996-14
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 36 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F4A29

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 0 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Title : VOC Analysis

37	7.385	1867	1880	1892	rBV2	95409	197617	15.17%	1.422%
38	7.571	1924	1938	1949	rBV	173200	309101	23.73%	2.225%
39	7.636	1951	1958	1971	rVV3	23508	51493	3.95%	0.371%
40	7.700	1972	1978	1990	rVB5	12665	22846	1.75%	0.164%
41	7.771	1991	2000	2012	rVB7	8594	17343	1.33%	0.125%
42	7.903	2014	2041	2055	rBV	599848	1048753	80.52%	7.548%
43	8.051	2073	2087	2099	rBV4	16143	39197	3.01%	0.282%
44	8.182	2117	2128	2141	rVB	112405	189990	14.59%	1.367%
45	8.372	2172	2187	2193	rVV4	13194	26257	2.02%	0.189%
46	8.414	2194	2200	2212	rVV2	16686	29531	2.27%	0.213%
47	8.494	2216	2225	2238	rVV2	12844	23571	1.81%	0.170%
48	8.555	2238	2244	2250	rVB3	1447	1692	0.13%	0.012%
49	8.639	2256	2270	2286	rBV	526938	934379	71.73%	6.725%
50	8.723	2289	2296	2311	rVB	90834	162004	12.44%	1.166%
51	9.083	2398	2408	2413	rBV7	4432	8801	0.68%	0.063%
52	9.169	2427	2435	2455	rVB2	19733	37840	2.91%	0.272%
53	9.276	2458	2468	2478	rBV2	12793	20927	1.61%	0.151%
54	9.340	2478	2488	2499	rBV3	16407	29203	2.24%	0.210%
55	9.420	2500	2513	2529	rBV	536324	892324	68.51%	6.422%
56	9.613	2560	2573	2584	rVB9	7446	17207	1.32%	0.124%
57	9.694	2589	2598	2608	rVV2	9741	15727	1.21%	0.113%
58	9.764	2613	2620	2630	rVV4	7774	12343	0.95%	0.089%
59	9.822	2630	2638	2648	rVB6	3137	5790	0.44%	0.042%
60	9.986	2680	2689	2696	rVV5	2131	3859	0.30%	0.028%
61	10.028	2696	2702	2712	rVV6	3067	5195	0.40%	0.037%
62	10.102	2712	2725	2733	rVB5	3297	6513	0.50%	0.047%
63	10.256	2757	2773	2791	rBV3	13696	37212	2.86%	0.268%
64	10.485	2838	2844	2854	rVB2	11335	17382	1.33%	0.125%
65	10.549	2854	2864	2880	rBV2	29408	54567	4.19%	0.393%
66	10.758	2918	2929	2944	rVB	444569	712148	54.67%	5.125%
67	10.906	2969	2975	2979	rBV7	2652	3524	0.27%	0.025%
68	11.063	3017	3024	3026	rBV4	1705	1908	0.15%	0.014%
69	11.253	3074	3083	3088	rBV5	2868	4460	0.34%	0.032%
70	11.295	3088	3096	3111	rVB	9743	15204	1.17%	0.109%
71	11.398	3119	3128	3132	rBV5	1532	2271	0.17%	0.016%
72	11.465	3138	3149	3159	rVB4	5978	10723	0.82%	0.077%
73	11.581	3178	3185	3187	rBV4	1088	1390	0.11%	0.010%
74	11.610	3188	3194	3200	rVV2	3539	5585	0.43%	0.040%
75	11.642	3200	3204	3212	rVB2	4279	5930	0.46%	0.043%
76	11.738	3228	3234	3245	rVB8	3961	6891	0.53%	0.050%

LSC Area Percent Report

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Acq On : 06 Oct 2021 00:20
Operator : SY/MD
Sample : M3996-14
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 36 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F4A29

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 0 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Title : VOC Analysis

77	11.816	3245	3258	3271	rBV	539791	866706	66.54%	6.238%
78	11.896	3275	3283	3296	rVB	39657	61037	4.69%	0.439%
79	12.099	3336	3346	3356	rBV4	15123	23563	1.81%	0.170%
80	12.195	3363	3376	3392	rVB	574388	920184	70.64%	6.623%
81	12.308	3405	3411	3423	rBV9	3772	6597	0.51%	0.047%
82	12.452	3451	3456	3463	rBV5	1103	1512	0.12%	0.011%
83	12.571	3487	3493	3501	rVB4	5927	7793	0.60%	0.056%
84	12.636	3507	3513	3519	rBV6	1225	1527	0.12%	0.011%
85	12.684	3519	3528	3544	rVB	40388	64780	4.97%	0.466%
86	12.880	3583	3589	3600	rVB4	2926	4068	0.31%	0.029%
87	12.973	3609	3618	3627	rBV	16593	23986	1.84%	0.173%
88	13.295	3709	3718	3726	rBV2	1825	2816	0.22%	0.020%
89	13.459	3758	3769	3780	rVV3	35932	60541	4.65%	0.436%
90	13.523	3780	3789	3798	rVB2	15472	23637	1.81%	0.170%
91	13.629	3813	3822	3831	rVB3	5482	8002	0.61%	0.058%
92	13.793	3862	3873	3881	rBV5	2635	4589	0.35%	0.033%
93	13.893	3897	3904	3905	rBV2	2355	2084	0.16%	0.015%
94	14.089	3954	3965	3979	rBV	66172	103861	7.97%	0.748%
95	14.211	3994	4003	4012	rVB2	11974	17814	1.37%	0.128%
96	14.626	4121	4132	4137	rBV4	1081	1975	0.15%	0.014%
97	14.732	4157	4165	4179	rBV4	2735	3992	0.31%	0.029%
98	14.812	4183	4190	4196	rBV4	1360	1641	0.13%	0.012%
99	15.169	4294	4301	4312	rBV2	5543	8313	0.64%	0.060%
100	15.414	4366	4377	4389	rBV2	24931	42249	3.24%	0.304%

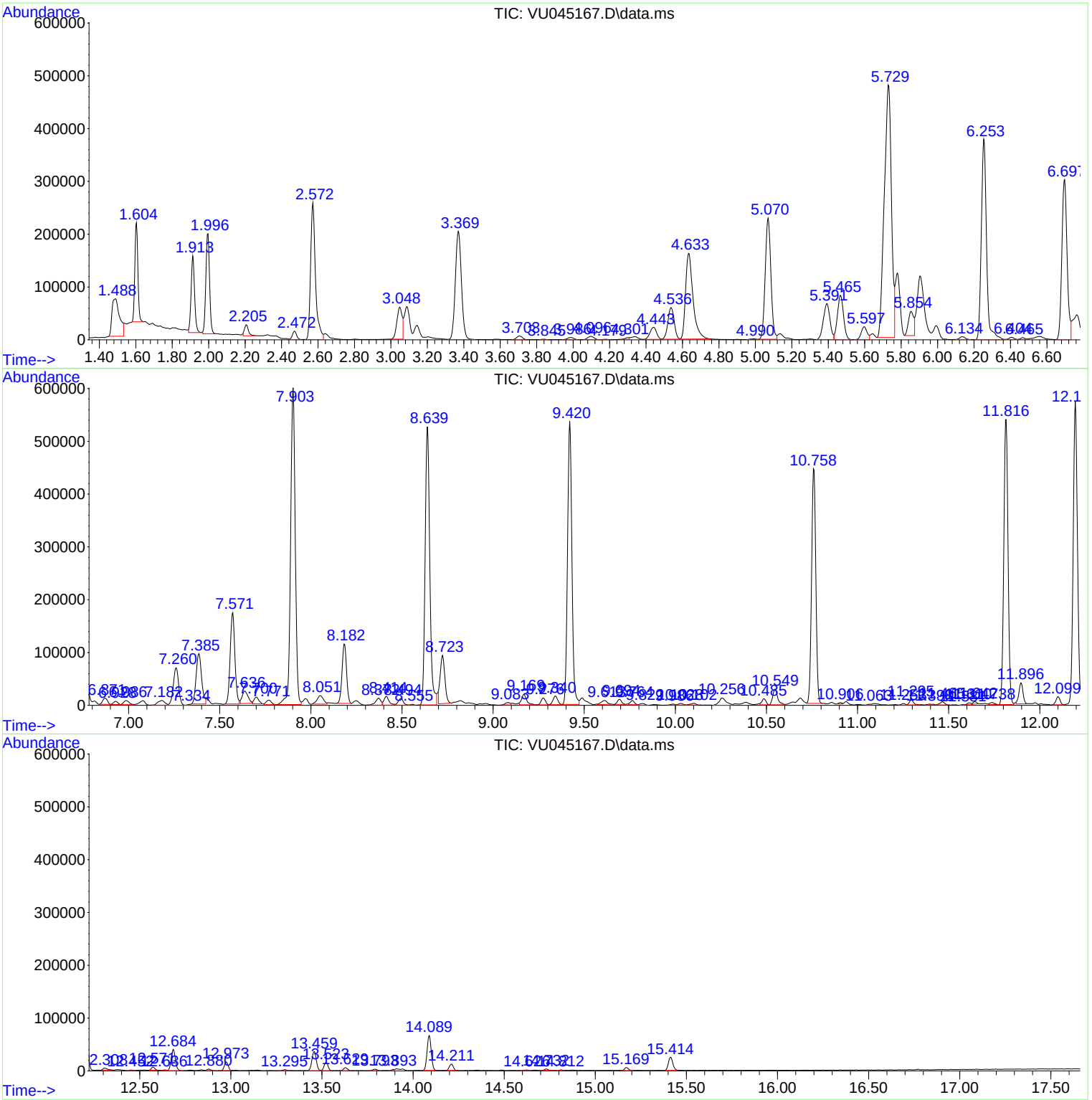
Sum of corrected areas: 13894314

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100521\
Data File : VU045167.D
Acq On : 06 Oct 2021 00:20
Operator : SY/MD
Sample : M3996-14
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 36 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F4A29

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100521\
Data File : VU045167.D
Acq On : 06 Oct 2021 00:20
Operator : SY/MD
Sample : M3996-14
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 36 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F4A29

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

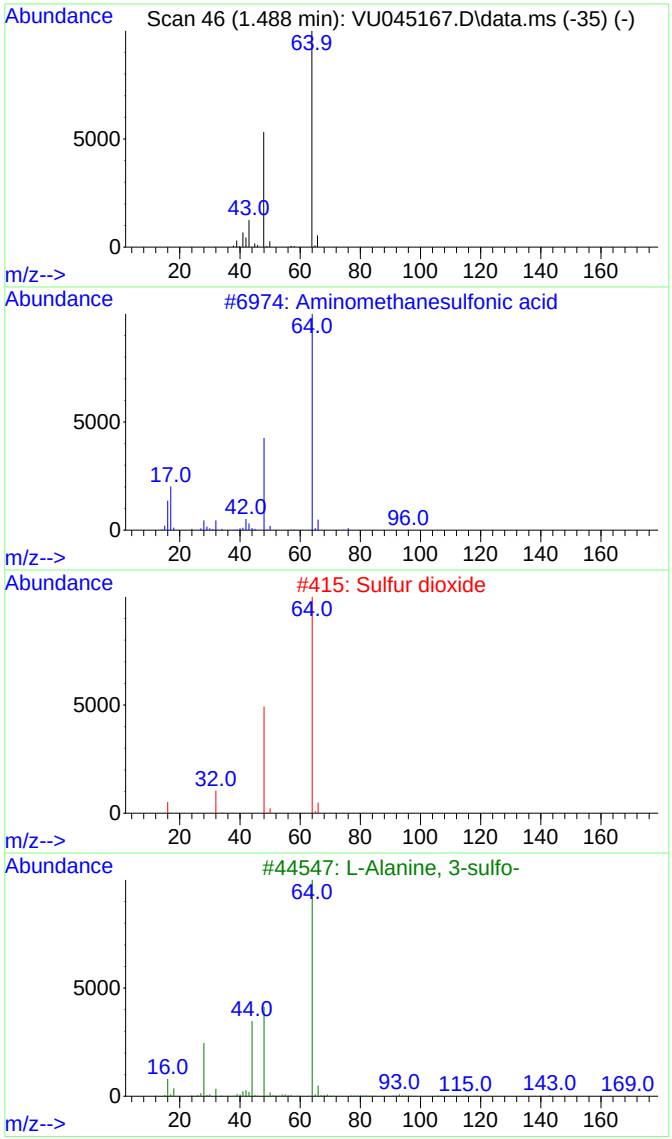
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

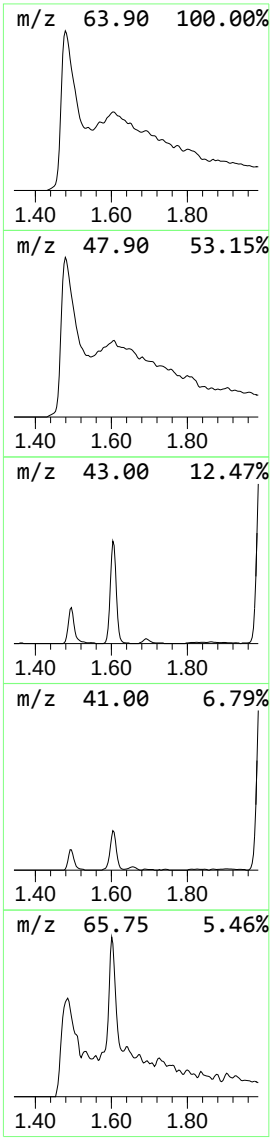
****

Peak Number 1 Aminomethanesulfonic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.488	13.67 ug/L	206746	1,4-Difluorobenzene	6.253

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	83
2	Sulfur dioxide	64	O2S	007446-09-5	83
3	L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	64
4	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
5	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100521\
Data File : VU045167.D
Acq On : 06 Oct 2021 00:20
Operator : SY/MD
Sample : M3996-14
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 36 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F4A29

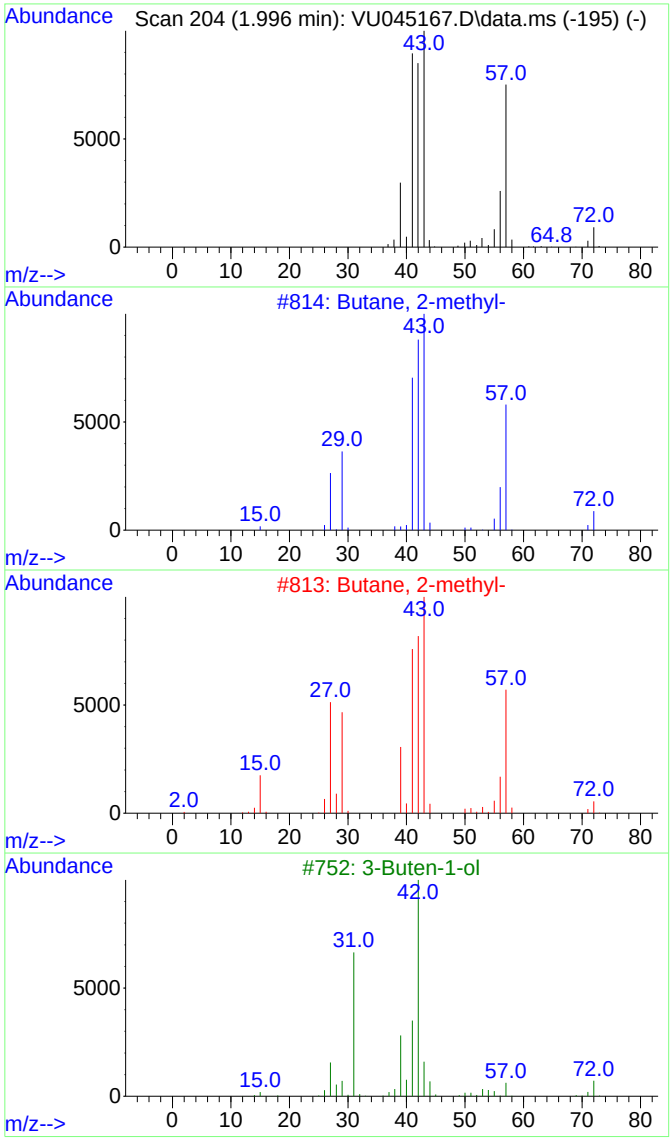
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

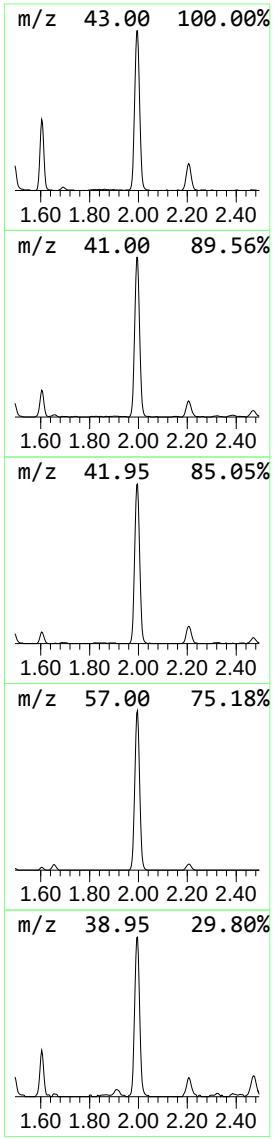
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.996	17.53 ug/L	265261	1,4-Difluorobenzene	6.253

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	87
2	Butane, 2-methyl-	72	C5H12	000078-78-4	86
3	3-Buten-1-ol	72	C4H8O	000627-27-0	37
4	Pentane	72	C5H12	000109-66-0	28
5	1-Butene	56	C4H8	000106-98-9	11





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100521\
Data File : VU045167.D
Acq On : 06 Oct 2021 00:20
Operator : SY/MD
Sample : M3996-14
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 36 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F4A29

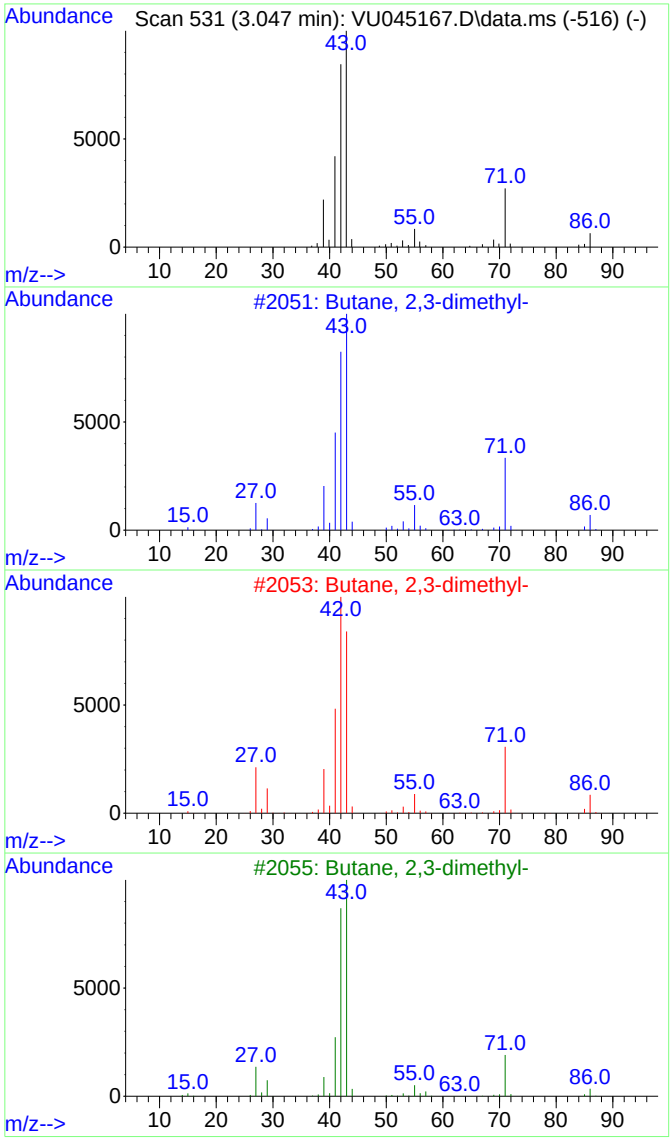
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

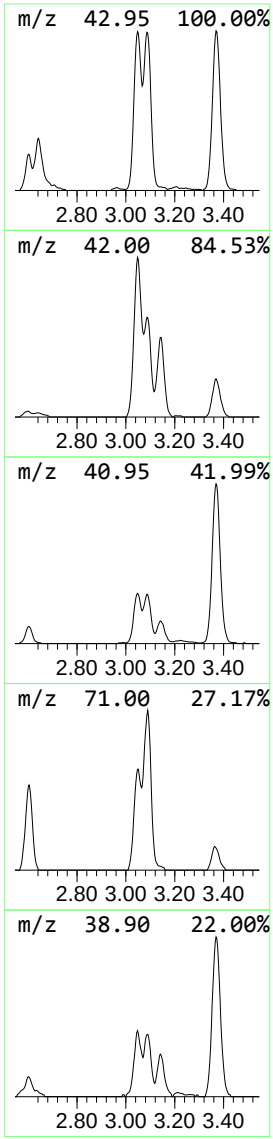
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.047	8.22 ug/L	124345	1,4-Difluorobenzene	6.253

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	90
2	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	87
3	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	86
4	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	86
5	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	80





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ALS Vial : 36 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F4A29

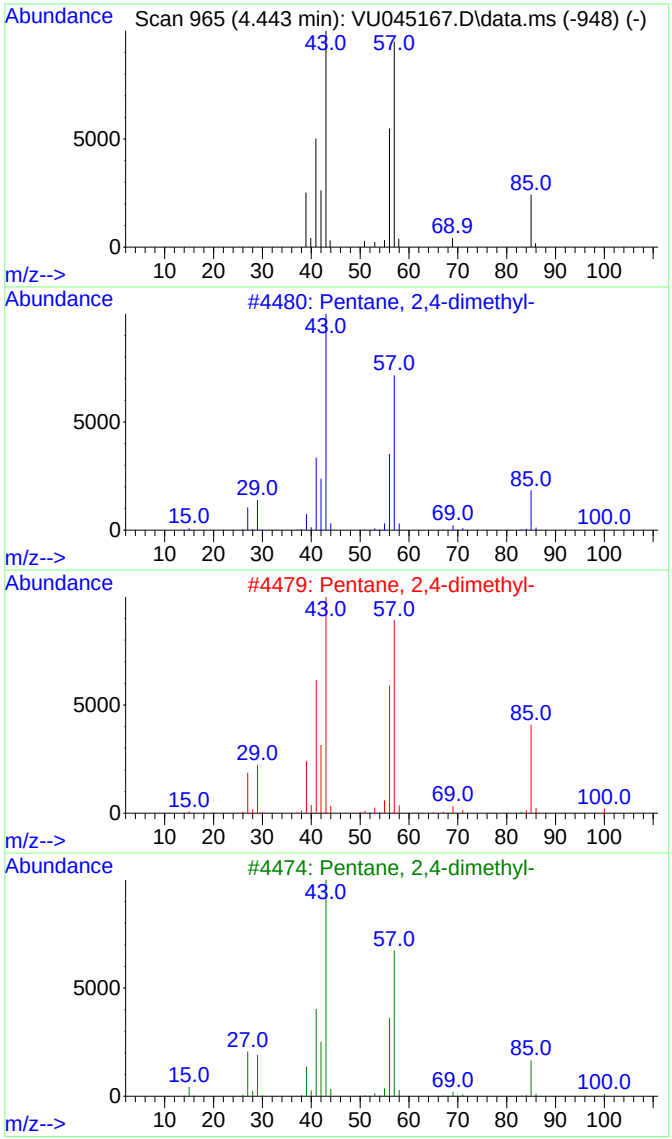
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

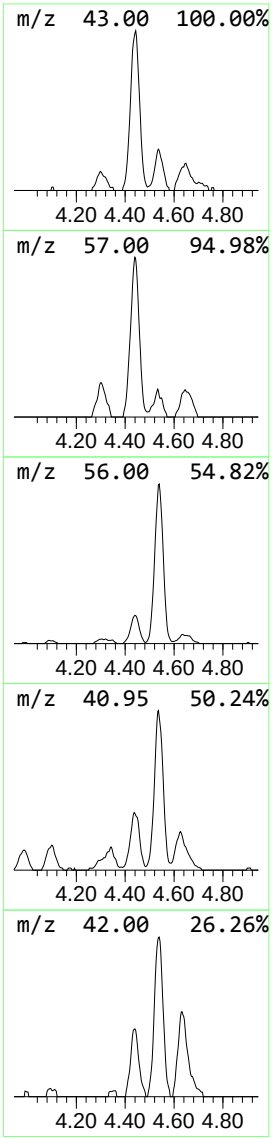
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.443	3.75 ug/L	56735	1,4-Difluorobenzene	6.253

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,4-dimethyl-	100	C7H16	000108-08-7	83
2	Pentane, 2,4-dimethyl-	100	C7H16	000108-08-7	74
3	Pentane, 2,4-dimethyl-	100	C7H16	000108-08-7	74
4	Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	64
5	Heptane, 3-methyl-	114	C8H18	000589-81-1	50





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100521\
Data File : VU045167.D
Acq On : 06 Oct 2021 00:20
Operator : SY/MD
Sample : M3996-14
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 36 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F4A29

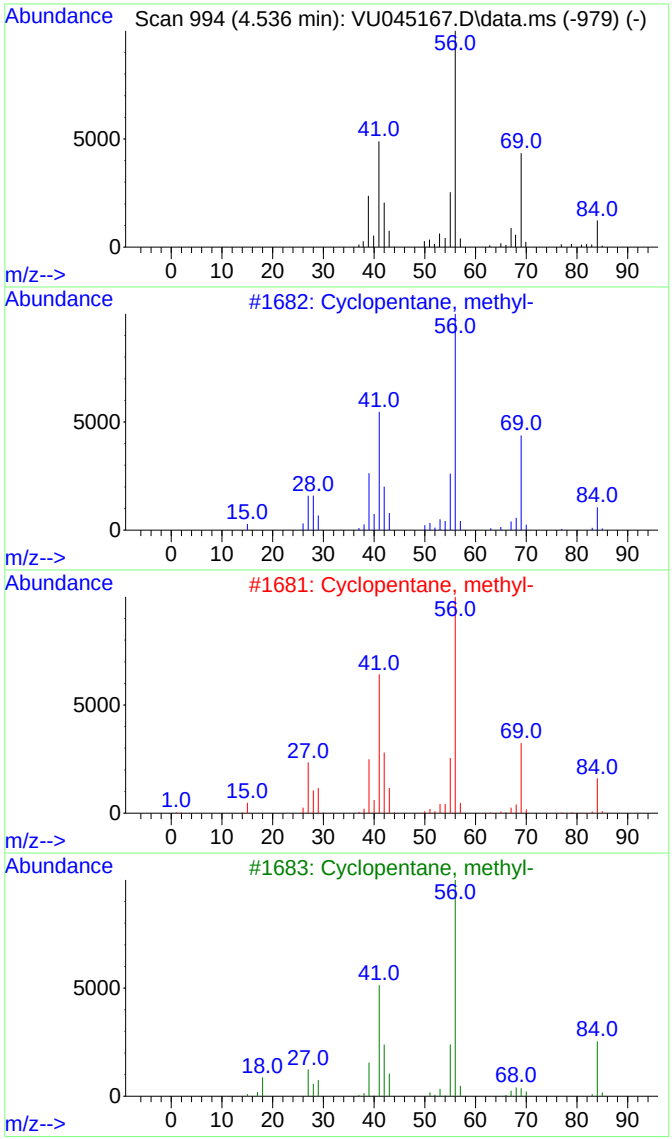
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

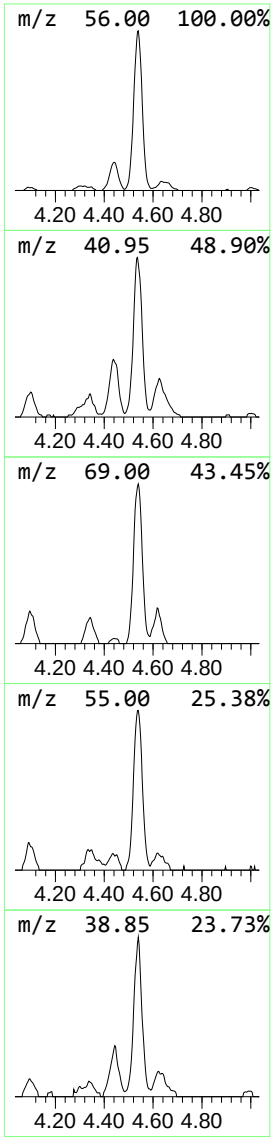
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 (DEL) Alkane: Cyclic4.536 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.536	9.42 ug/L	142457	1,4-Difluorobenzene	6.253

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	91
2	Cyclopentane, methyl-	84	C6H12	000096-37-7	87
3	Cyclopentane, methyl-	84	C6H12	000096-37-7	72
4	Cyclobutane, ethyl-	84	C6H12	004806-61-5	72
5	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	64





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Data File : VU045167.D
Acq On : 06 Oct 2021 00:20
Operator : SY/MD
Sample : M3996-14
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 36 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F4A29

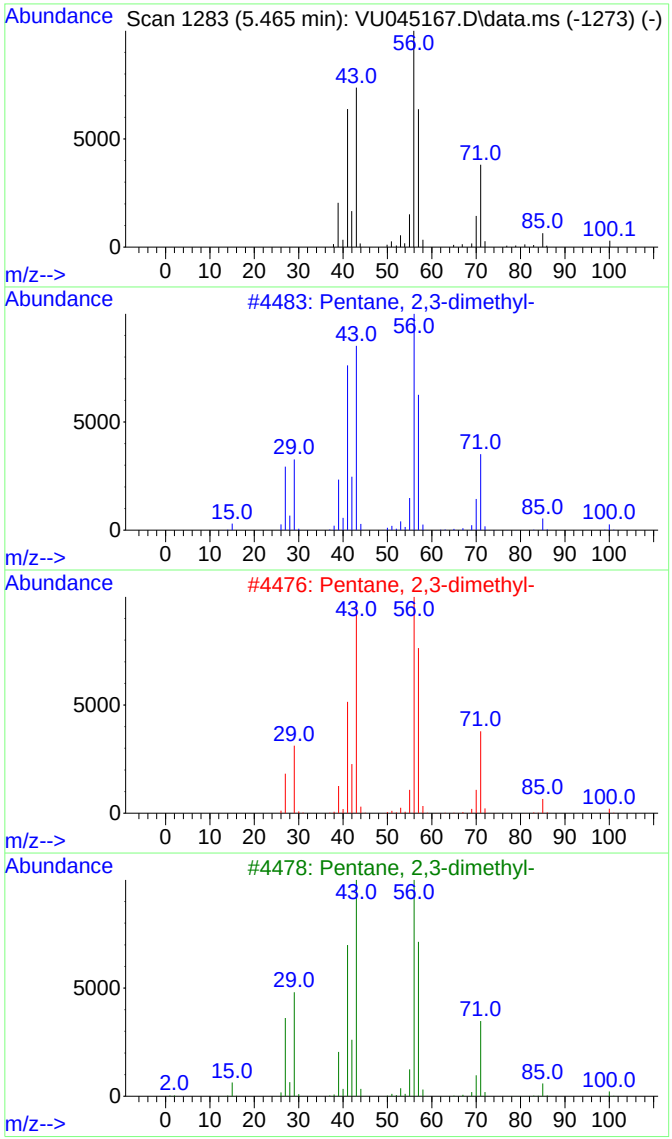
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

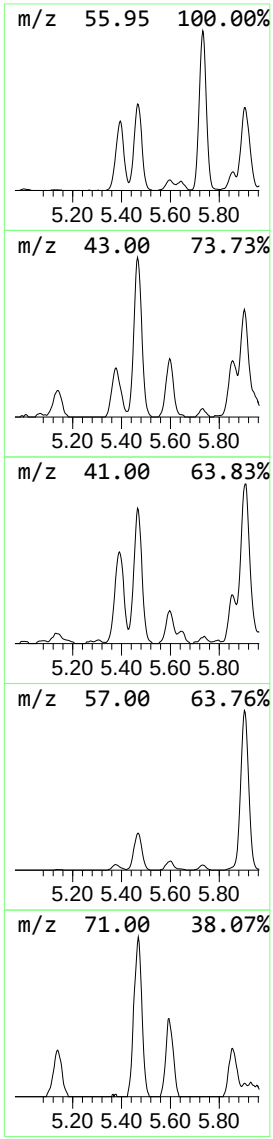
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.465	12.76 ug/L	192995	1,4-Difluorobenzene	6.253

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	91
2	Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	91
3	Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	83
4	Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	74
5	Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	45





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Acq On : 06 Oct 2021 00:20
Operator : SY/MD
Sample : M3996-14
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 36 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F4A29

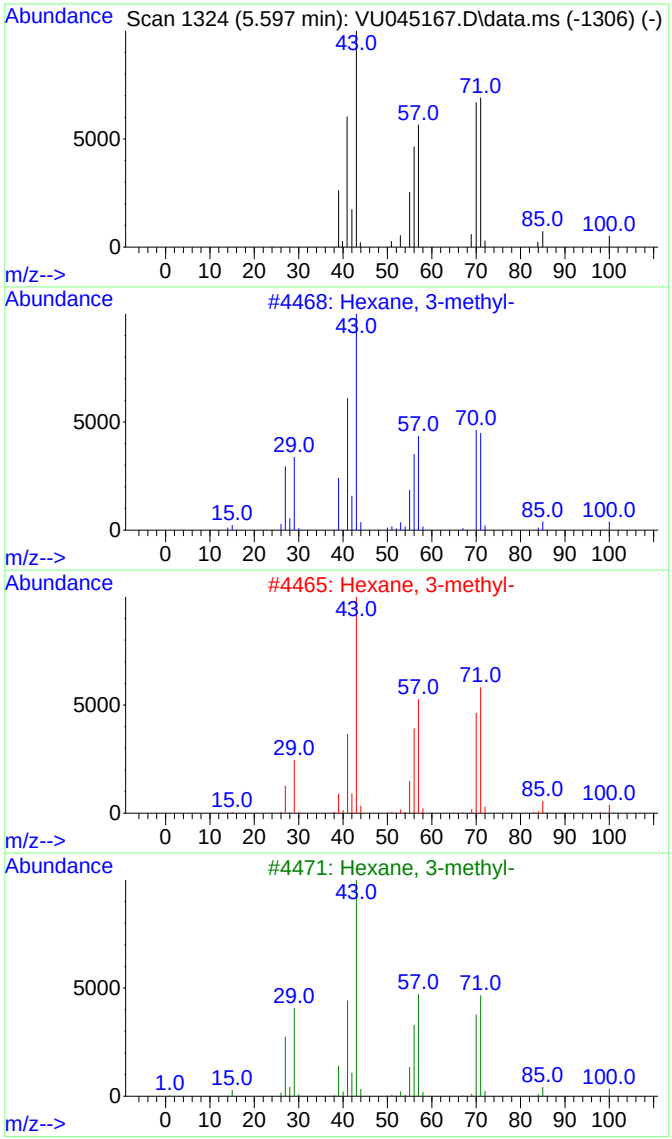
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

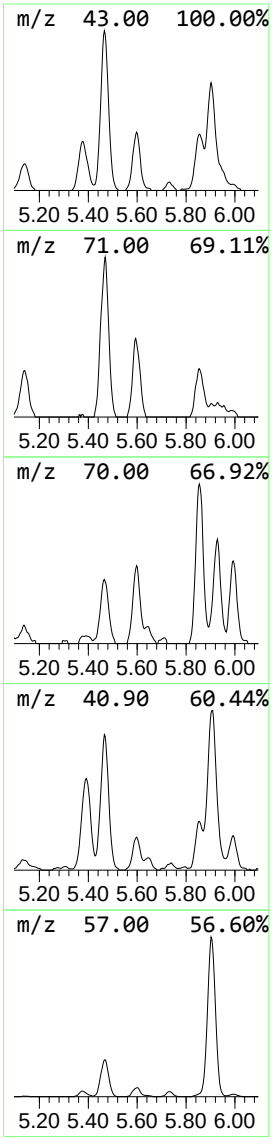
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 (DEL) Alkane: Straight-Chai... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.597	3.65 ug/L	55163	1,4-Difluorobenzene	6.253

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 3-methyl-	100	C7H16	000589-34-4	91
2	Hexane, 3-methyl-	100	C7H16	000589-34-4	90
3	Hexane, 3-methyl-	100	C7H16	000589-34-4	83
4	Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	53
5	Heptane, 3,4-dimethyl-	128	C9H20	000922-28-1	50





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Data File : VU045167.D
Acq On : 06 Oct 2021 00:20
Operator : SY/MD
Sample : M3996-14
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 36 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F4A29

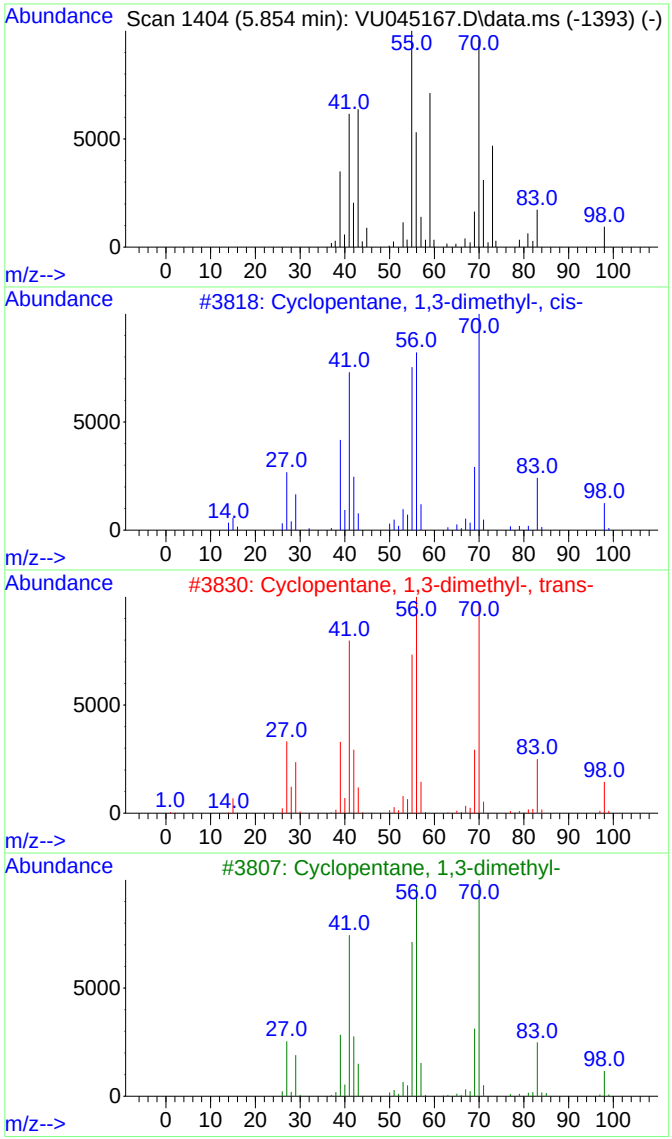
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

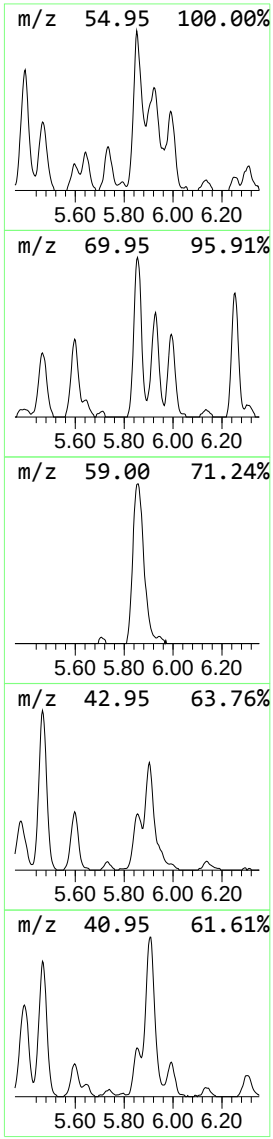
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 (DEL) Alkane: Cyclic5.854 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.854	6.29 ug/L	95210	1,4-Difluorobenzene	6.253

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, 1,3-dimethyl-, cis-	98	C7H14	002532-58-3	55
2	Cyclopentane, 1,3-dimethyl-, trans-	98	C7H14	001759-58-6	46
3	Cyclopentane, 1,3-dimethyl-	98	C7H14	002453-00-1	43
4	1-Butanol, 3-methyl-, acetate	130	C7H14O2	000123-92-2	43
5	Cyclopentane, 1,2-dimethyl-, cis-	98	C7H14	001192-18-3	43





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Acq On : 06 Oct 2021 00:20
Operator : SY/MD
Sample : M3996-14
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 36 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F4A29

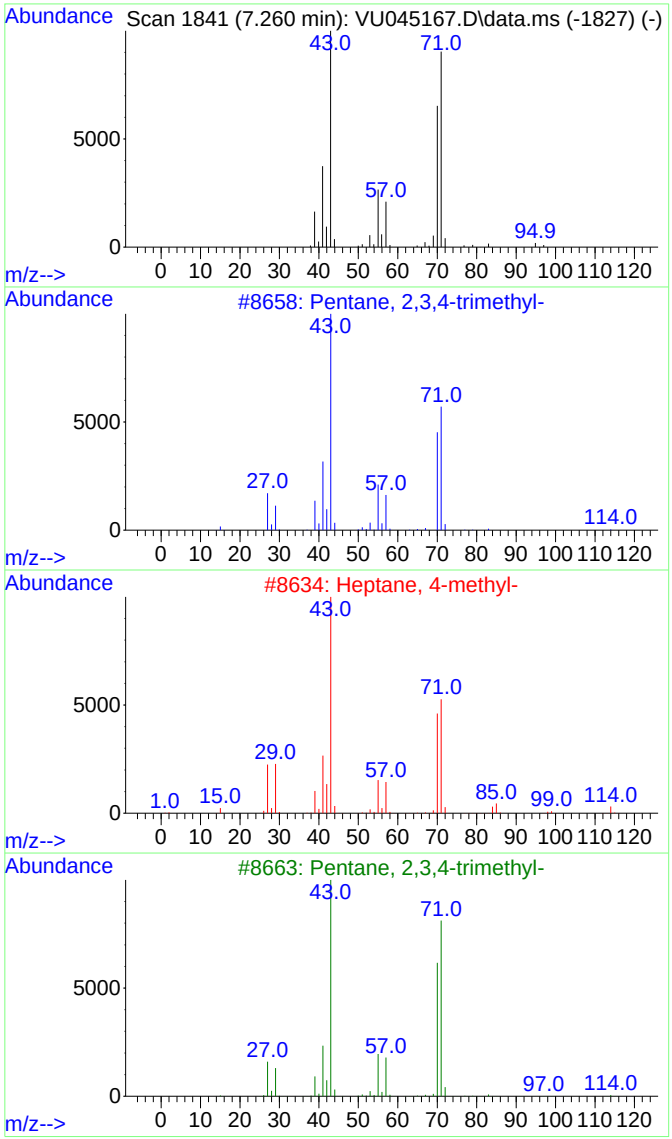
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

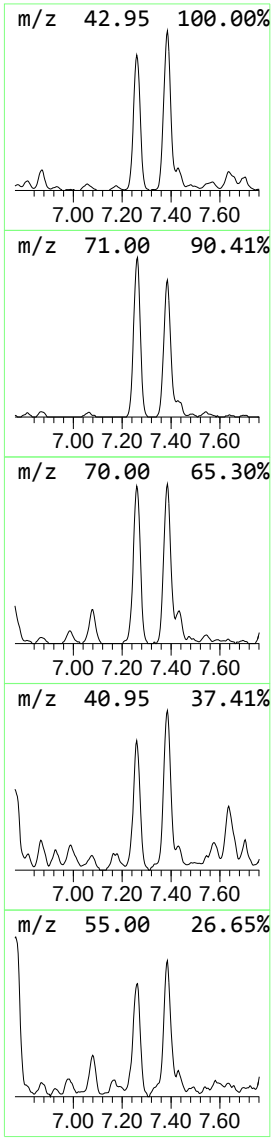
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 (DEL) Alkane: Straight-Chai... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.260	9.44 ug/L	142761	1,4-Difluorobenzene	6.253

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	90
2	Heptane, 4-methyl-	114	C8H18	000589-53-7	83
3	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	83
4	Heptane, 4-methyl-	114	C8H18	000589-53-7	83
5	Pentane, 3-ethyl-	100	C7H16	000617-78-7	74





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Acq On : 06 Oct 2021 00:20
Operator : SY/MD
Sample : M3996-14
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 36 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F4A29

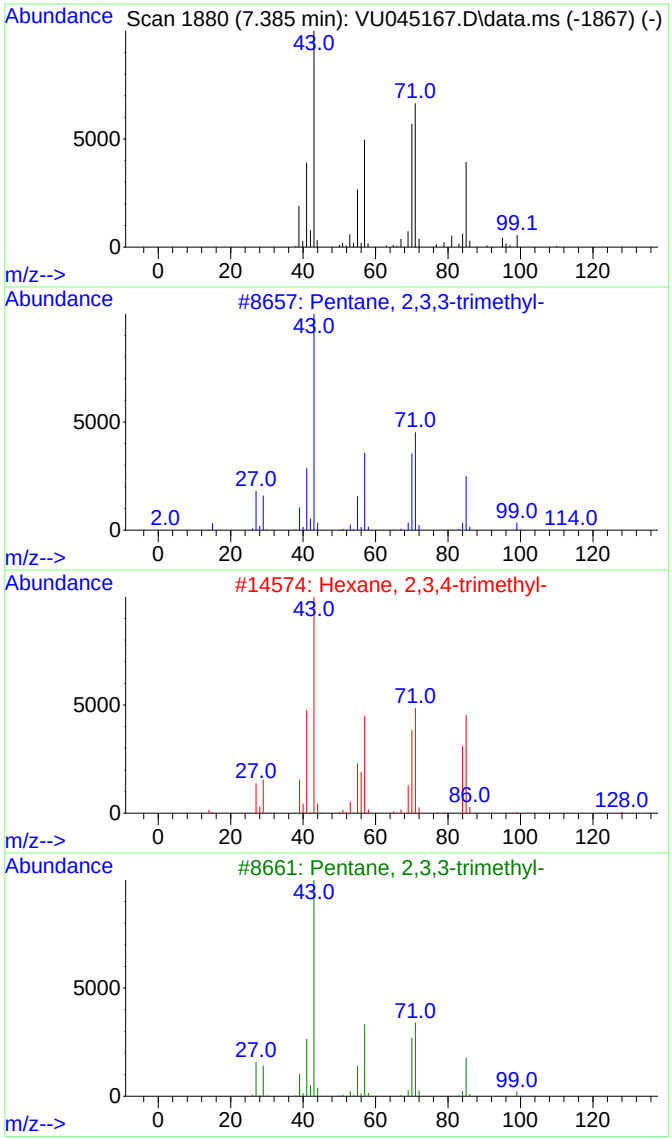
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

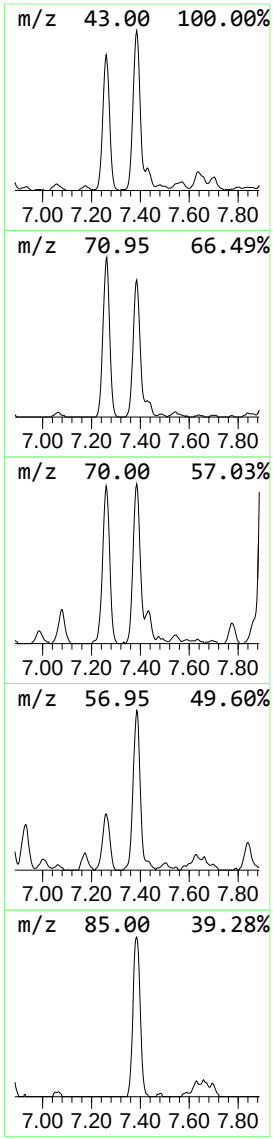
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.385	13.06 ug/L	197617	1,4-Difluorobenzene	6.253

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	90
2	Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	78
3	Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	72
4	Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	59
5	Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	59





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Data File : VU045167.D
Acq On : 06 Oct 2021 00:20
Operator : SY/MD
Sample : M3996-14
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 36 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F4A29

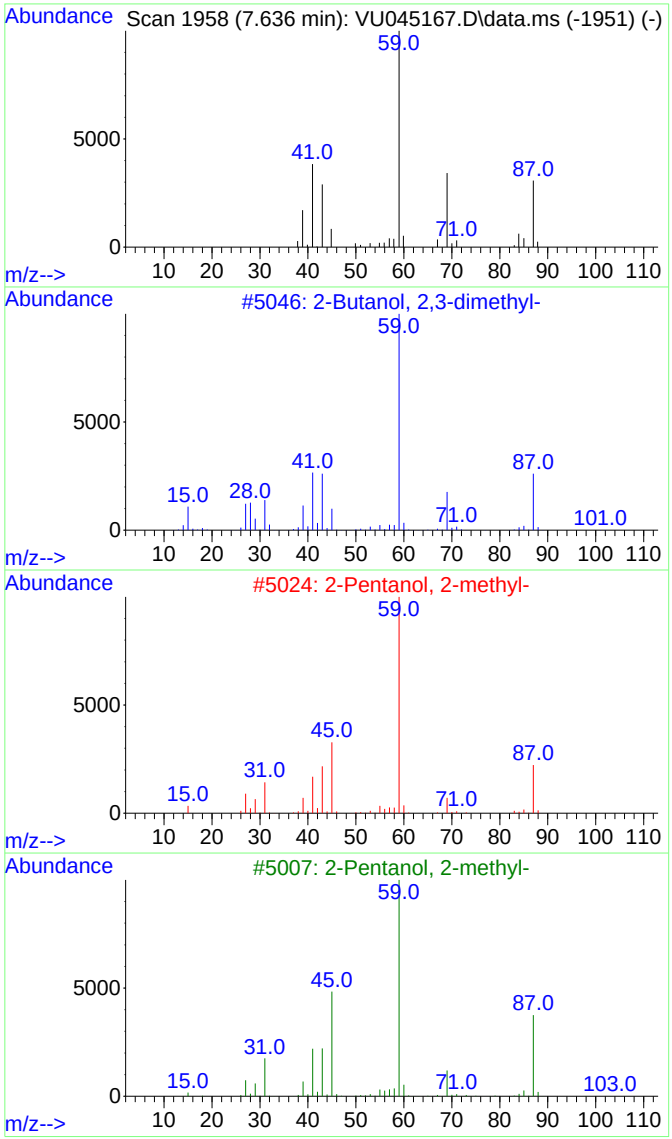
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

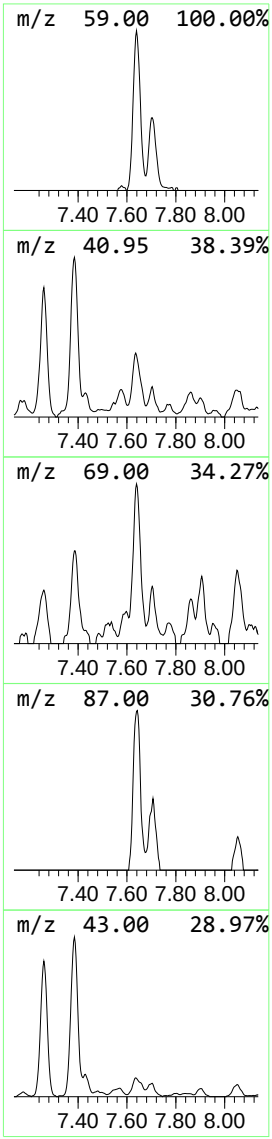
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 12 2-Butanol, 2,3-dimethyl- Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.636	3.40 ug/L	51493	1,4-Difluorobenzene	6.253

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanol, 2,3-dimethyl-	102	C6H14O	000594-60-5	83
2	2-Pentanol, 2-methyl-	102	C6H14O	000590-36-3	78
3	2-Pentanol, 2-methyl-	102	C6H14O	000590-36-3	74
4	2-Butanol, 2,3-dimethyl-	102	C6H14O	000594-60-5	64
5	2-Butanol, 2,3-dimethyl-	102	C6H14O	000594-60-5	64





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Data File : VU045167.D
Acq On : 06 Oct 2021 00:20
Operator : SY/MD
Sample : M3996-14
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 36 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F4A29

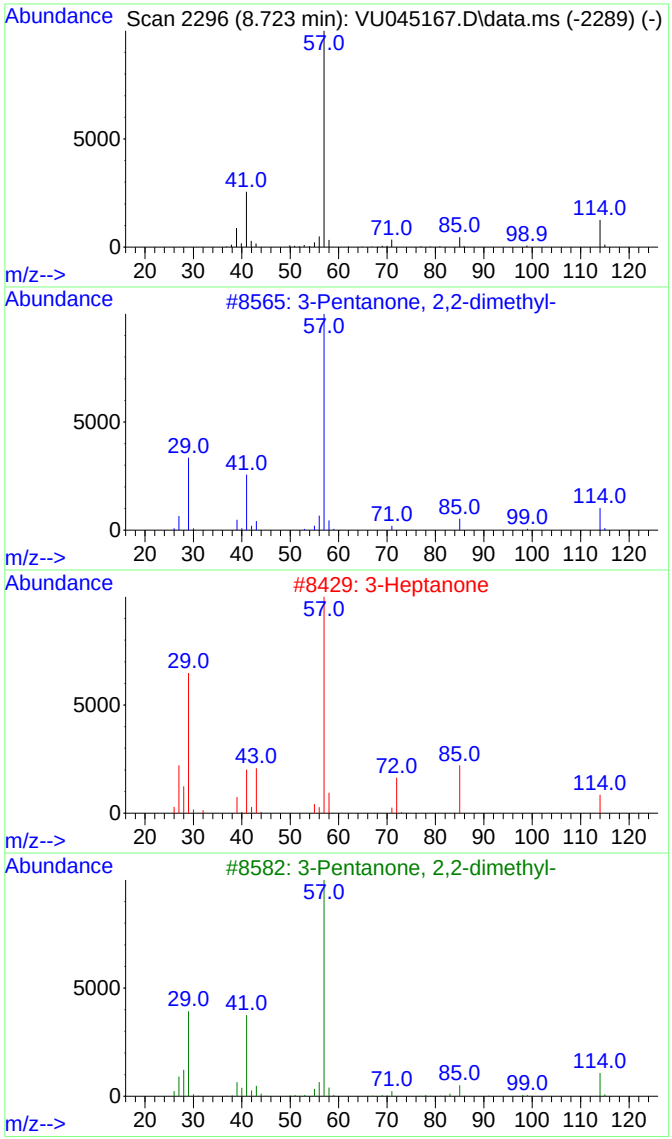
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

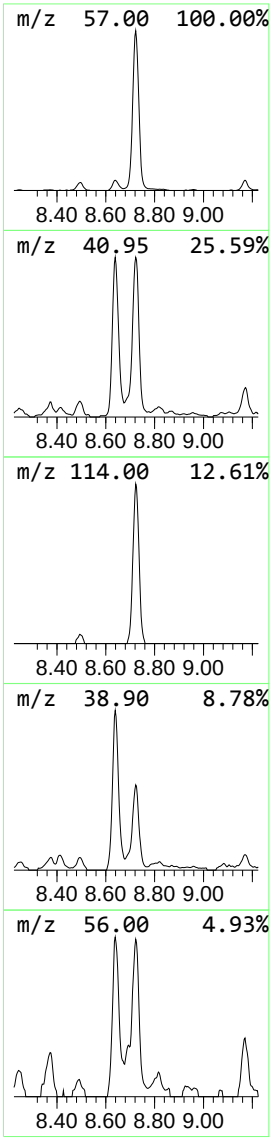
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 13 3-Pentanone, 2,2-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.723	9.08 ug/L	162004	Chlorobenzene-d5	9.420

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanone, 2,2-dimethyl-	114	C7H14O	000564-04-5	80
2	3-Heptanone	114	C7H14O	000106-35-4	53
3	3-Pentanone, 2,2-dimethyl-	114	C7H14O	000564-04-5	50
4	3,4-Hexanedione	114	C6H10O2	004437-51-8	50
5	Aluminum, triethyl-	114	C6H15Al	000097-93-8	42





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Acq On : 06 Oct 2021 00:20
Operator : SY/MD
Sample : M3996-14
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 36 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F4A29

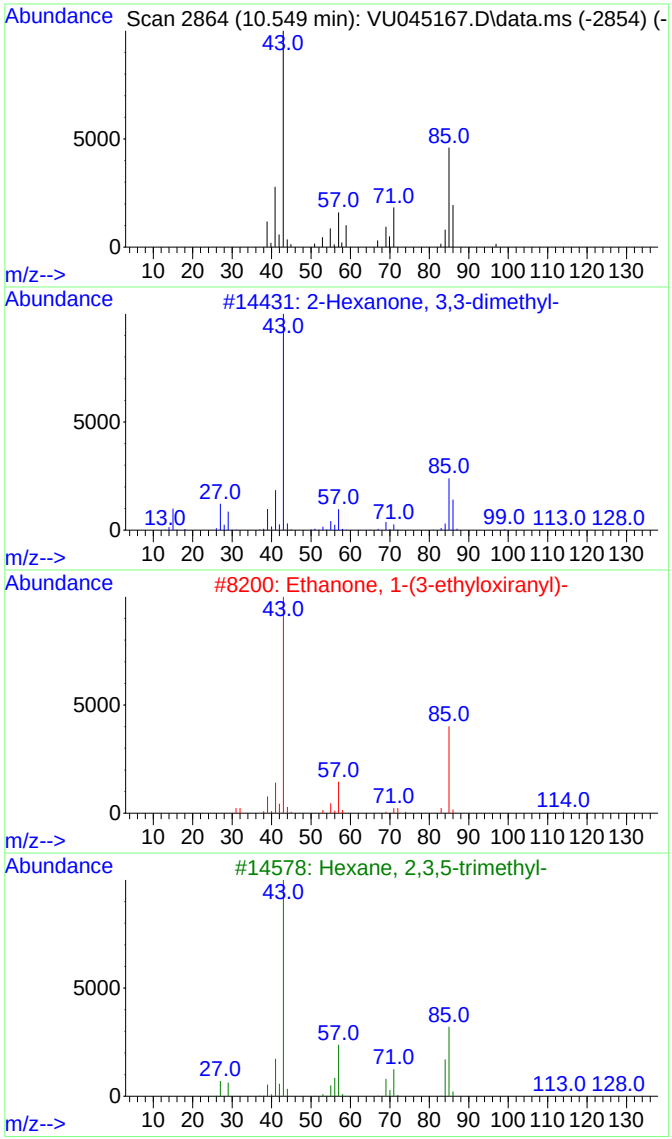
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

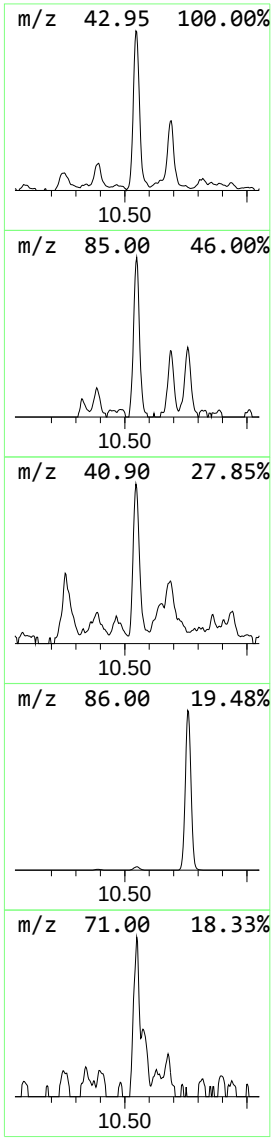
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 14 2-Hexanone, 3,3-dimethyl- Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.549	3.06 ug/L	54567	Chlorobenzene-d5	9.420

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hexanone, 3,3-dimethyl-	128	C8H16O	026118-38-7	64
2	Ethanone, 1-(3-ethyloxiranyl)-	114	C6H10O2	017257-81-7	43
3	Hexane, 2,3,5-trimethyl-	128	C9H20	001069-53-0	40
4	Hexane, 2,3,5-trimethyl-	128	C9H20	001069-53-0	40
5	Oxalic acid, diisohexyl ester	258	C14H26O4	1010309-32-9	40





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Operator : SY/MD
Sample : M3996-14
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 36 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F4A29

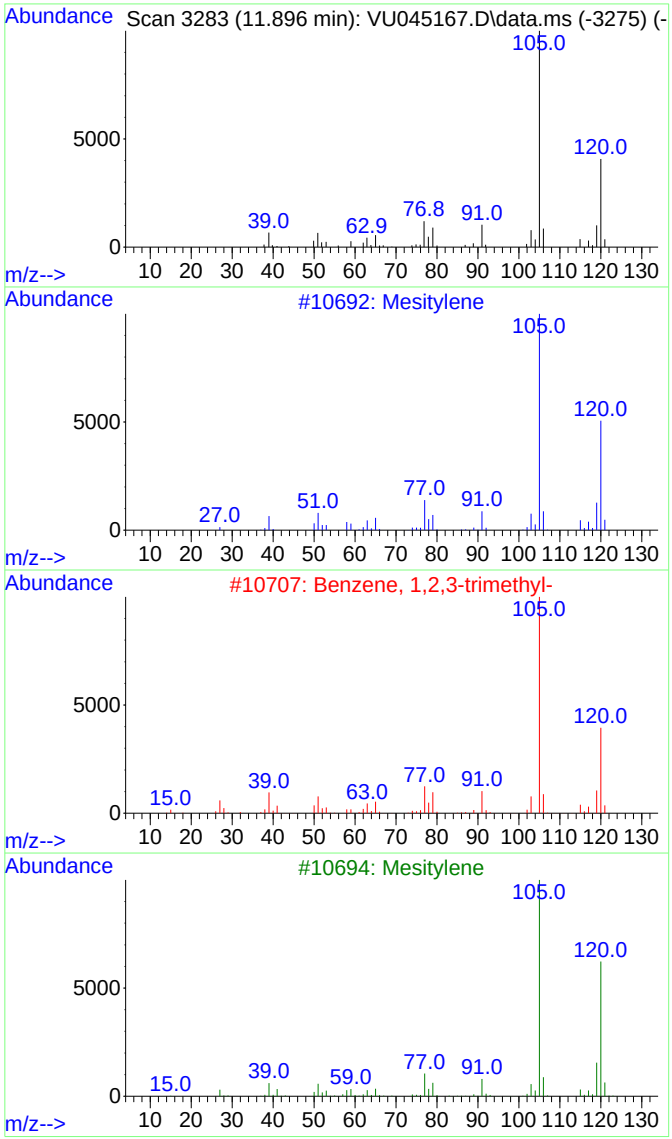
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

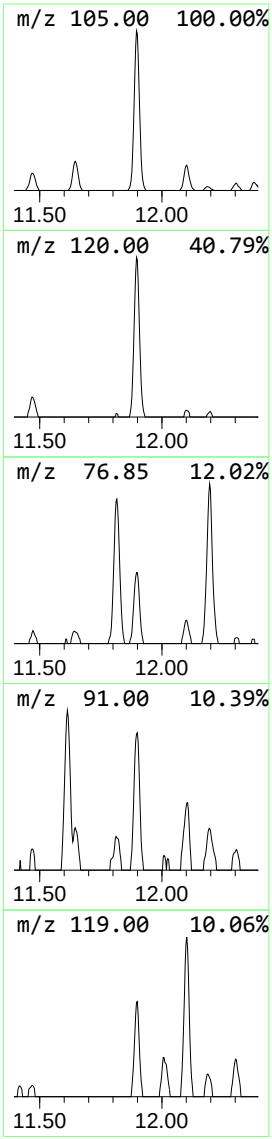
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 15 Benzene, 1,2,3-trimethyl- Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.896	3.52 ug/L	61037	1,4-Dichlorobenzene-d4	11.816

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Mesitylene	120	C9H12	000108-67-8	97
2	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	97
3	Mesitylene	120	C9H12	000108-67-8	94
4	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	94
5	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91





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Acq On : 06 Oct 2021 00:20
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Sample : M3996-14
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 36 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F4A29

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

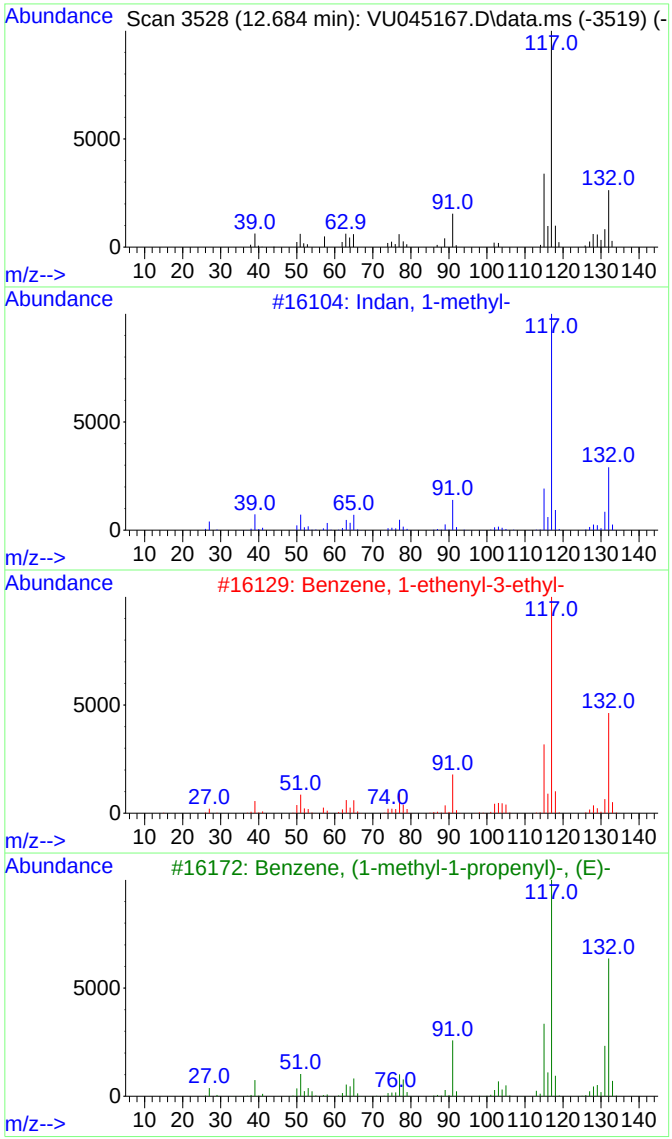
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

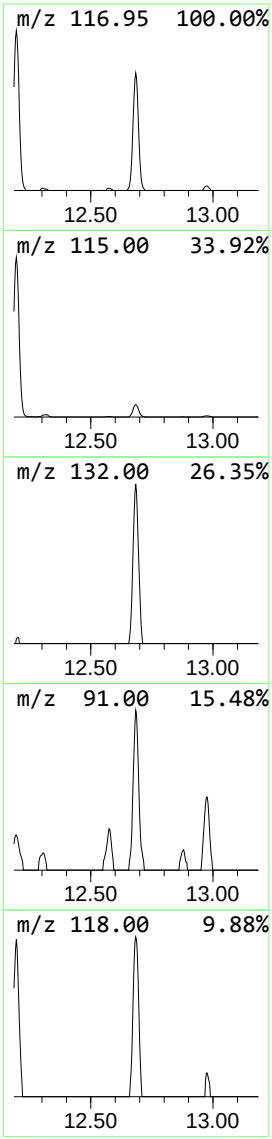
****

Peak Number 16 Indan, 1-methyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.684	3.74 ug/L	64780	1,4-Dichlorobenzene-d4	11.816

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indan, 1-methyl-	132	C10H12	000767-58-8	91
2	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	91
3	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	87
4	1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	86
5	Benzene, 2-butenyl-	132	C10H12	001560-06-1	86





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Operator : SY/MD
Sample : M3996-14
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 36 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F4A29

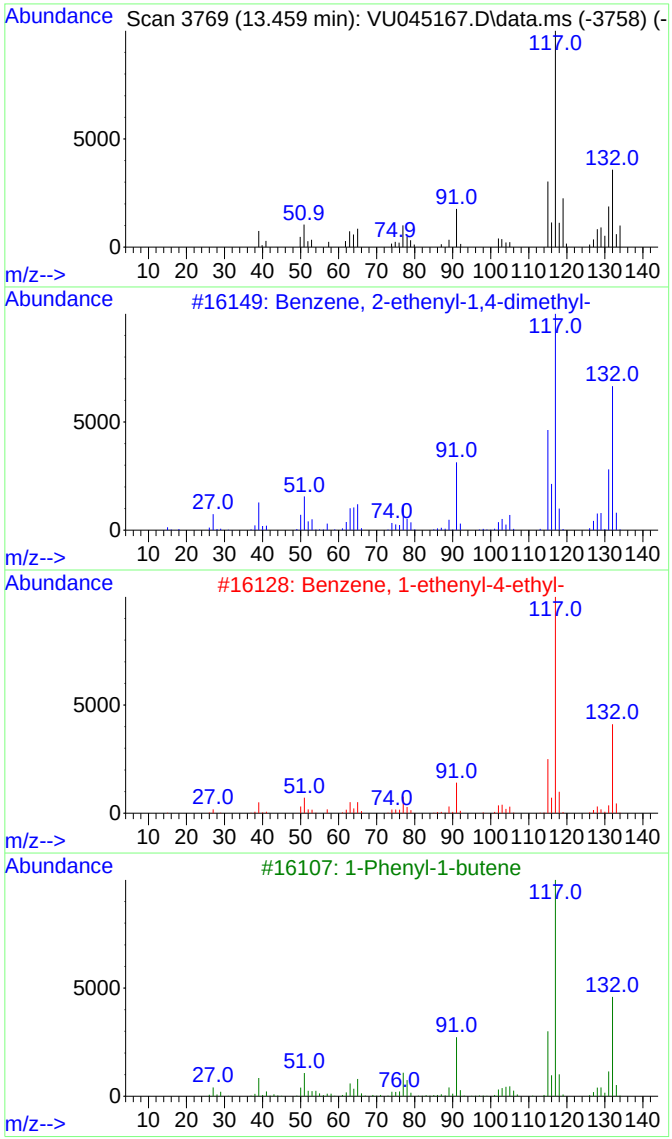
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

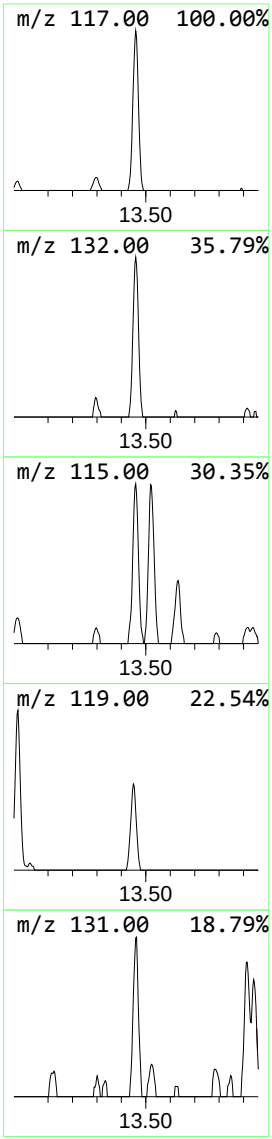
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 17 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.459	3.49 ug/L	60541	1,4-Dichlorobenzene-d4	11.816

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	96
2	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	94
3	1-Phenyl-1-butene	132	C10H12	000824-90-8	90
4	3-Phenylbut-1-ene	132	C10H12	000934-10-1	81
5	1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	76





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Data File : VU045167.D
Acq On : 06 Oct 2021 00:20
Operator : SY/MD
Sample : M3996-14
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 36 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F4A29

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

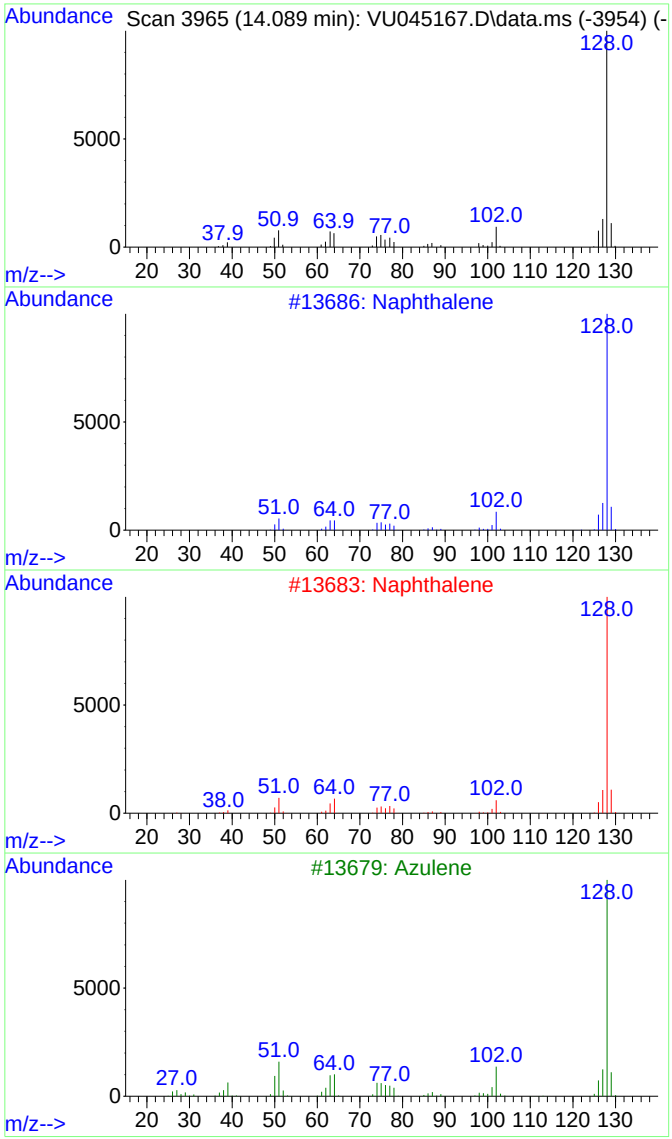
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

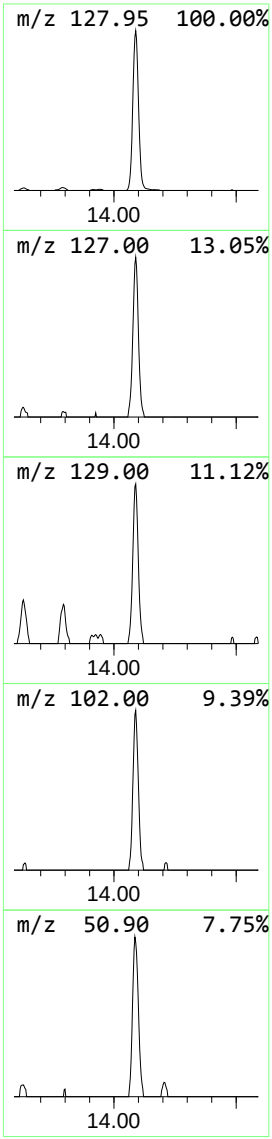
****

Peak Number 18 Azulene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.089	5.99 ug/L	103861	1,4-Dichlorobenzene-d4	11.816

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene	128	C10H8	000091-20-3	95
2	Naphthalene	128	C10H8	000091-20-3	95
3	Azulene	128	C10H8	000275-51-4	91
4	Azulene	128	C10H8	000275-51-4	91
5	Naphthalene	128	C10H8	000091-20-3	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100521\
Data File : VU045167.D
Acq On : 06 Oct 2021 00:20
Operator : SY/MD
Sample : M3996-14
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 36 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F4A29

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Aminomethanesul...	1.488	13.7	ug/L	206746	1	6.253	756421	50.0
(DEL) Alkane: S...	1.996	17.5	ug/L	265261	1	6.253	756421	50.0
(DEL) Alkane: S...	3.047	8.2	ug/L	124345	1	6.253	756421	50.0
(DEL) Alkane: S...	4.443	3.8	ug/L	56735	1	6.253	756421	50.0
(DEL) Alkane: C...	4.536	9.4	ug/L	142457	1	6.253	756421	50.0
(DEL) Alkane: S...	5.465	12.8	ug/L	192995	1	6.253	756421	50.0
(DEL) Alkane: S...	5.597	3.6	ug/L	55163	1	6.253	756421	50.0
(DEL) Alkane: C...	5.854	6.3	ug/L	95210	1	6.253	756421	50.0
(DEL) Alkane: S...	7.260	9.4	ug/L	142761	1	6.253	756421	50.0
(DEL) Alkane: S...	7.385	13.1	ug/L	197617	1	6.253	756421	50.0
2-Butanol, 2,3-...	7.636	3.4	ug/L	51493	1	6.253	756421	50.0
3-Pentanone, 2,...	8.723	9.1	ug/L	162004	2	9.420	892324	50.0
2-Hexanone, 3,3...	10.549	3.1	ug/L	54567	2	9.420	892324	50.0
Benzene, 1,2,3-...	11.896	3.5	ug/L	61037	3	11.816	866706	50.0
Indan, 1-methyl-	12.684	3.7	ug/L	64780	3	11.816	866706	50.0
Benzene, 2-ethe...	13.459	3.5	ug/L	60541	3	11.816	866706	50.0
Azulene	14.089	6.0	ug/L	103861	3	11.816	866706	50.0